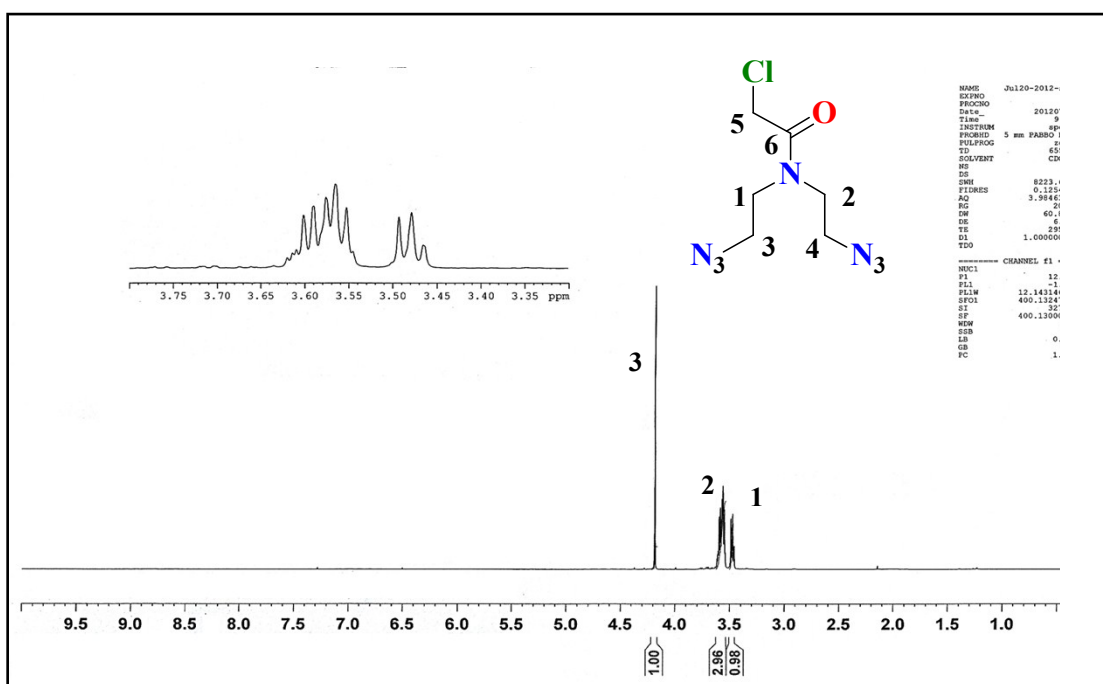


Supplementary Information

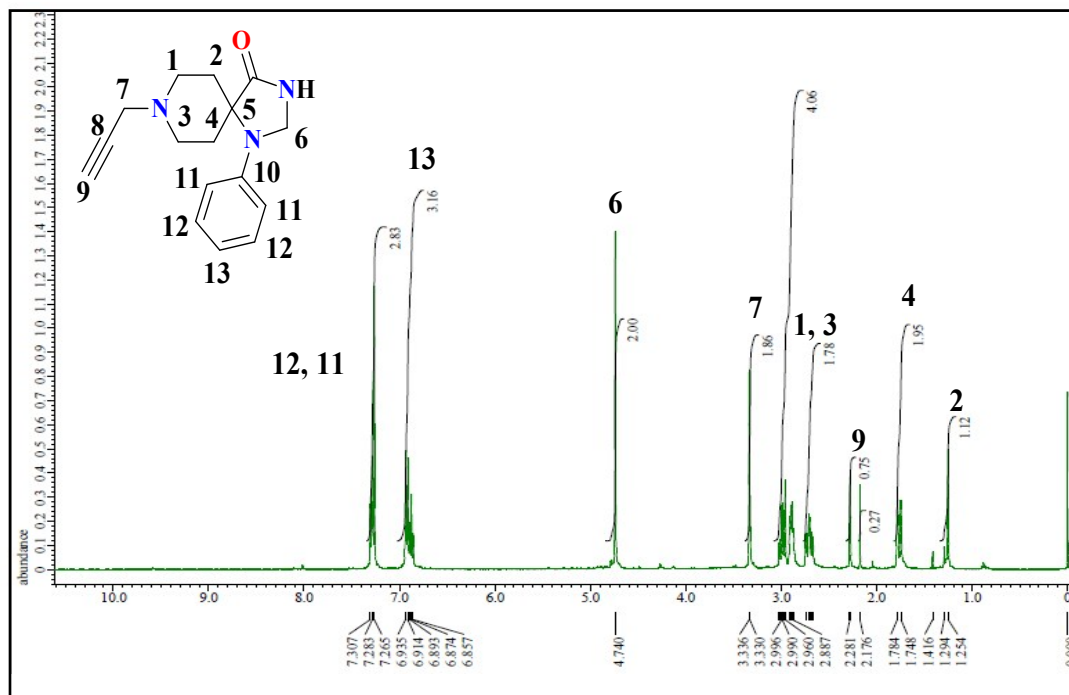
Design, Synthesis and Relaxation Studies of triazole linked Gadolinium(III)- DO3A-BT-bistriazaspirodecanone as a Potential MRI Contrast agent

Raunak Varshney,^a Swarndeeep K. Sethi,^{a,b} Sandhya Rangaswamy,^{a,b} Anjani K Tiwari, Ankur Kaul^a Marilyn D. Milton,^b Senthil Kumaran,^c Anil K. Mishra^{a*}

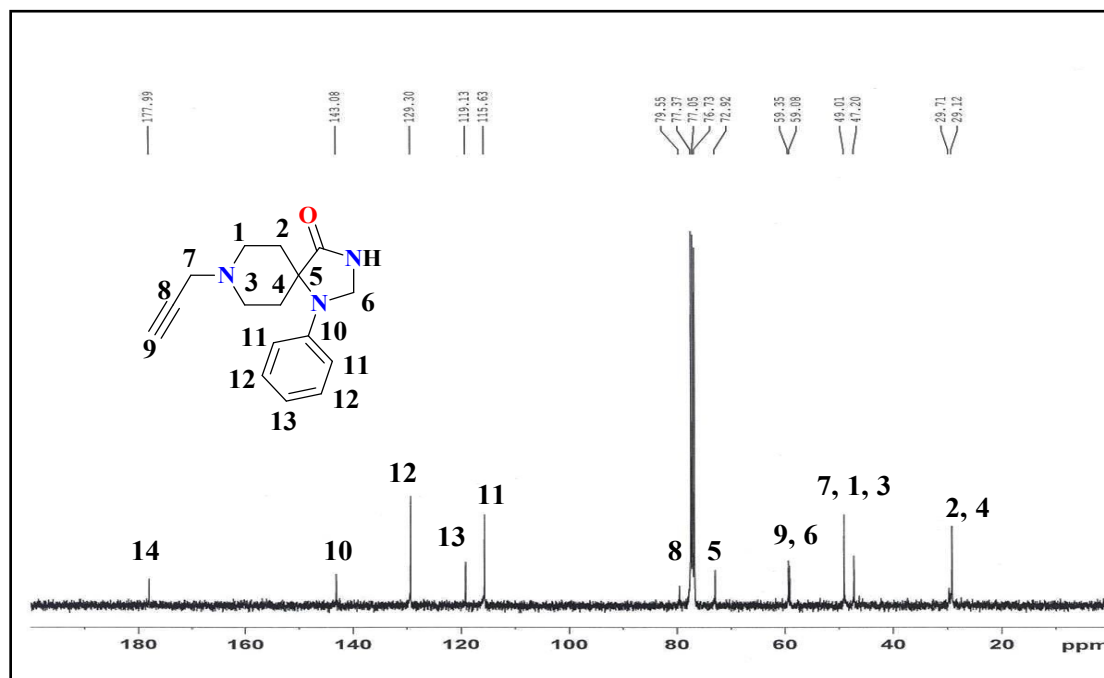
¹H NMR of N,N-bis(2-azidoethyl)-2-chloroacetamide (2) (Solvent: CDCl₃)



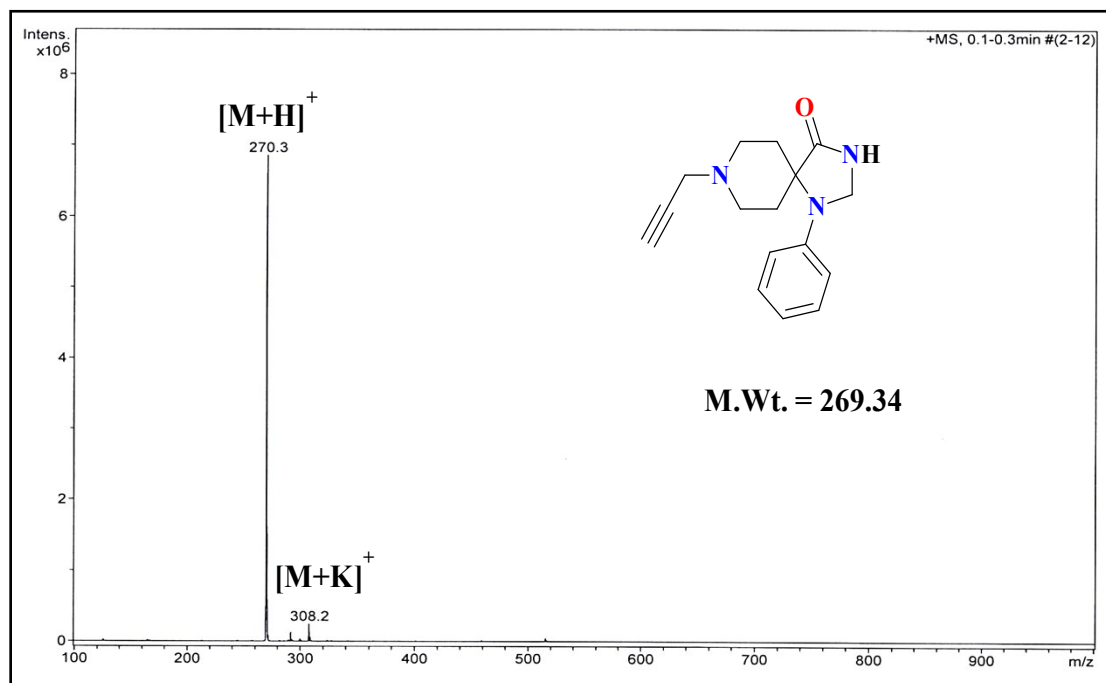
¹³C NMR of N,N-bis(2-azidoethyl)-2-chloroacetamide (2) (Solvent: CDCl₃)



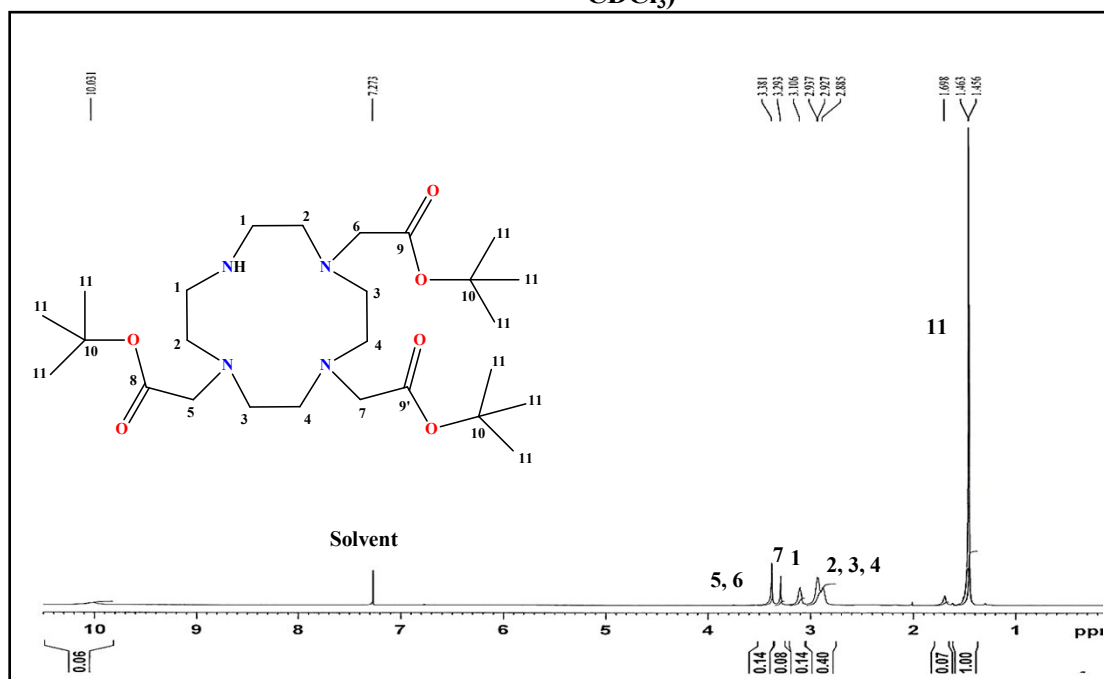
¹³C NMR of 1-phenyl-8-(prop-2-yn-1-yl)-1,3,8-triazaspiro[4,5]decan-4-one (4)
(Solvent: CDCl₃)



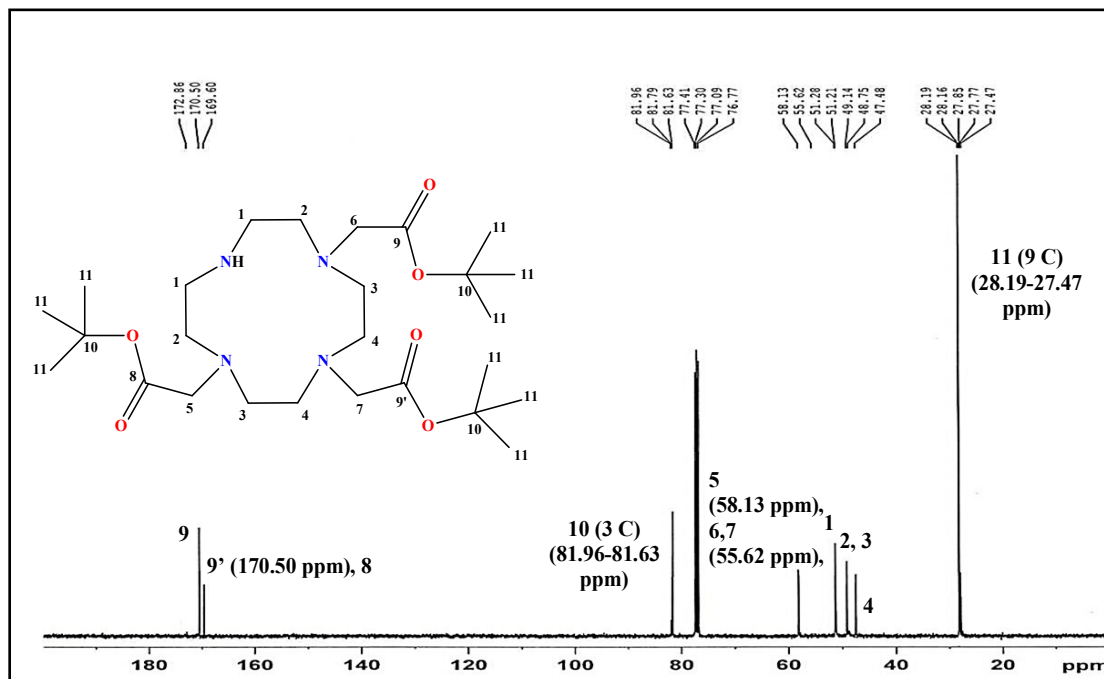
Mass Spectrum of 1-phenyl-8-(prop-2-yn-1-yl)-1,3,8-triazaspiro[4,5]decan-4-one (4)



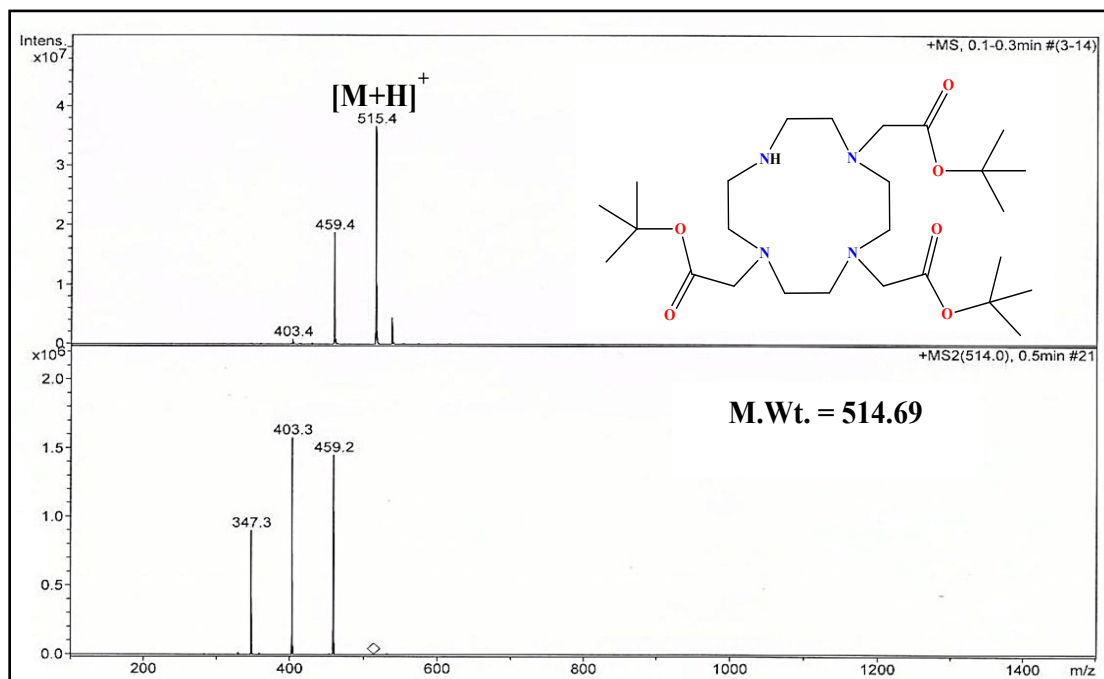
NMR of tri-tert-butyl 2,2',2''-(1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (6), (Solvent: CDCl₃)



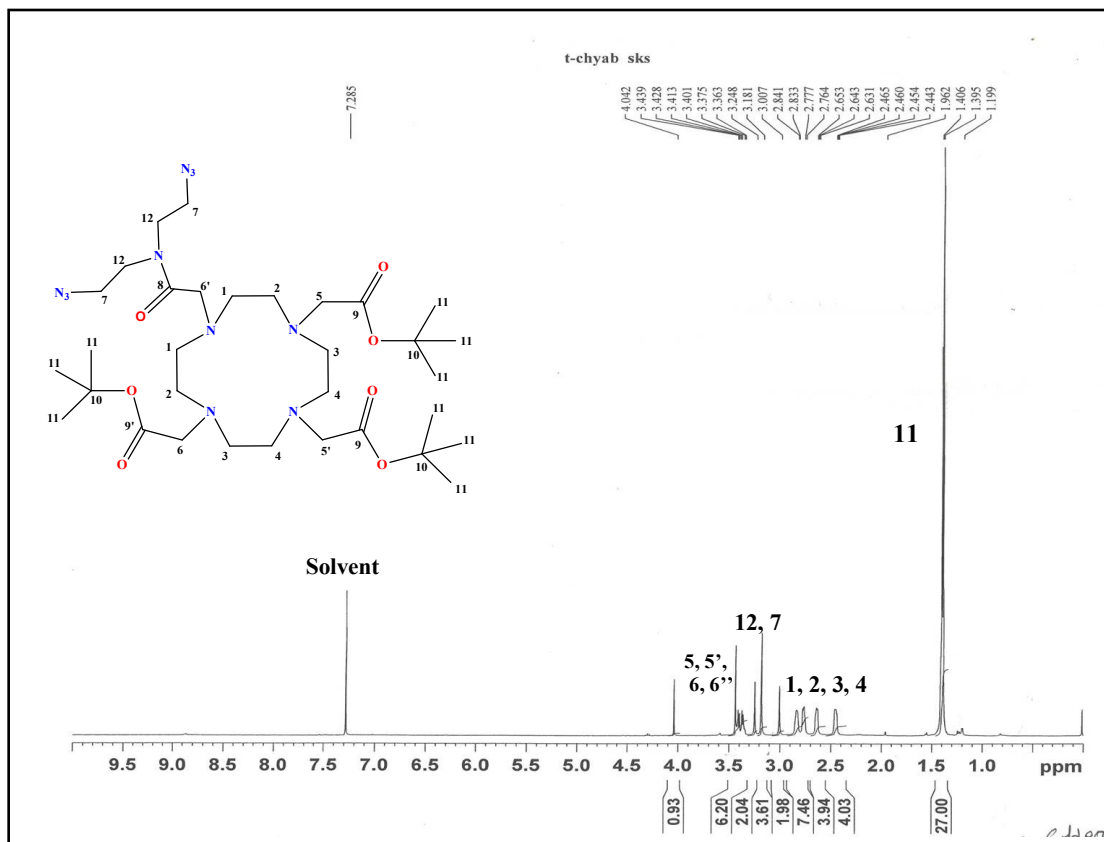
^{13}C NMR of tri-tert-butyl 2,2',2''-(1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (6), (Solvent: CDCl_3)



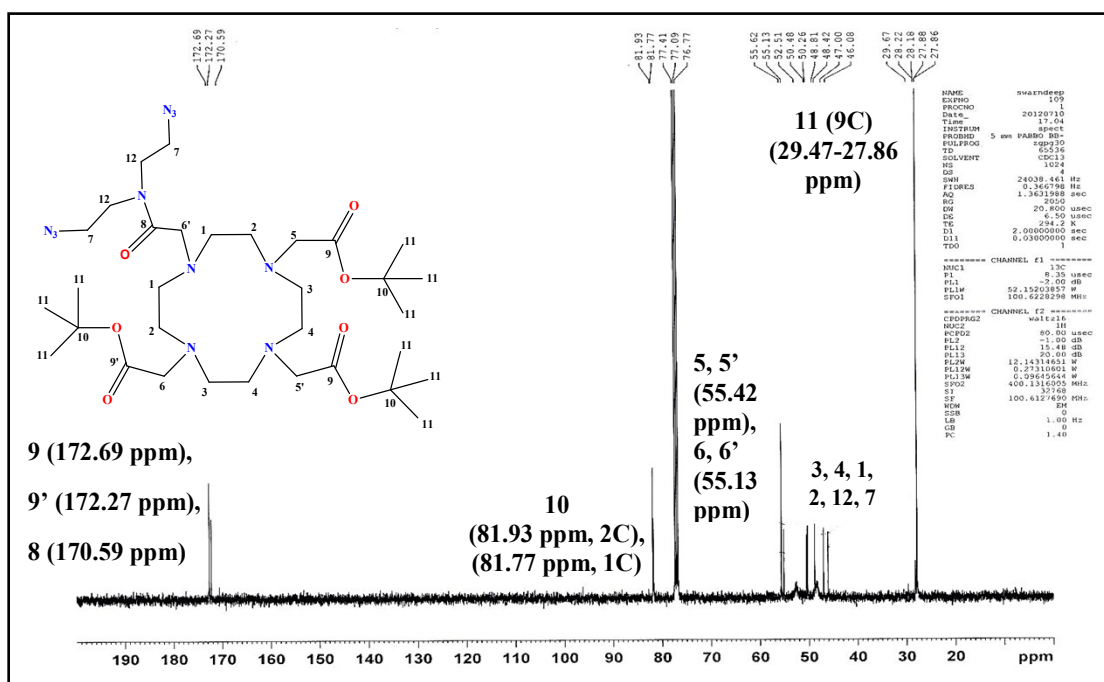
Mass Spectrum of tri-tert-butyl 2,2',2''-(1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (6)



^1H NMR of tri-tert-butyl 2,2',2''-(10-(3-(bis(2-azidoethyl)amino)-2-oxopropyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (7), (Solvent: CDCl_3)

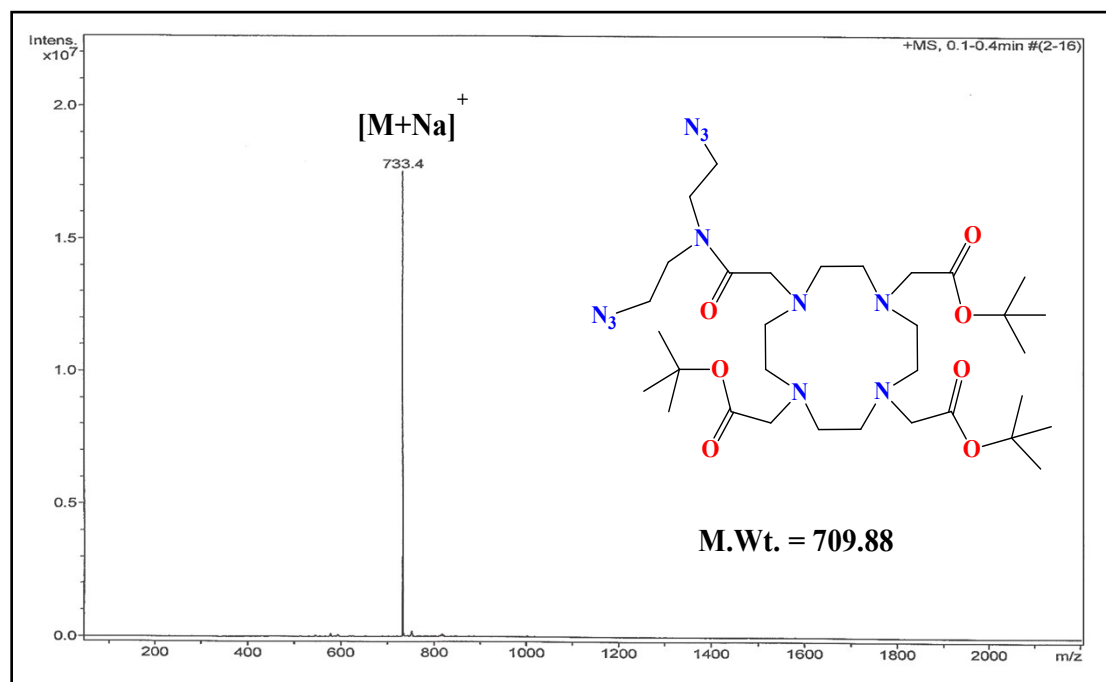


^{13}C NMR of tri-tert-butyl 2,2',2''-(10-(3-(bis(2-azidoethyl)amino)-2-oxopropyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (7), (Solvent: CDCl_3)

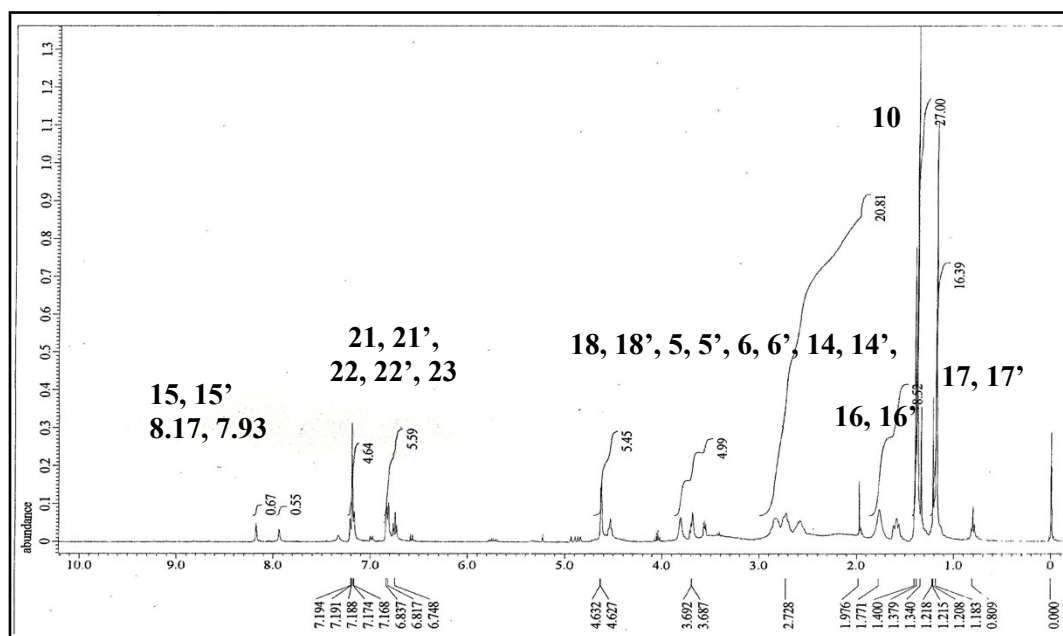
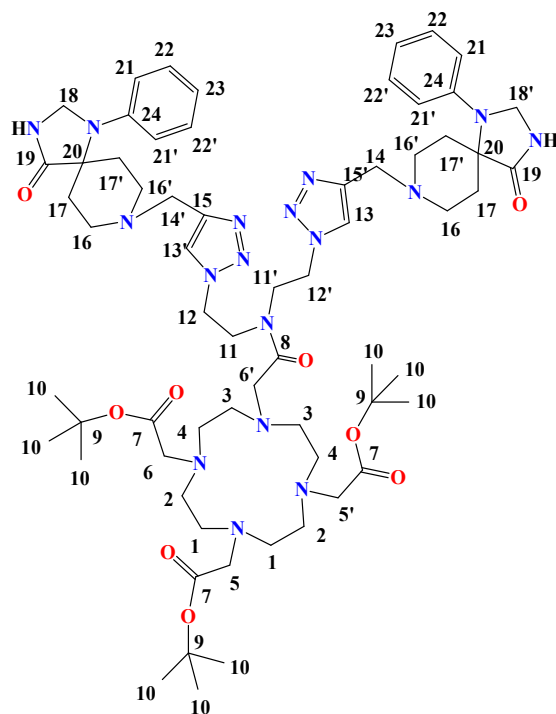


Values (ppm) = 3 (52.53 ppm), 4 (50.48, 50.26 ppm), 1 (48.81 ppm), 2 (48.42 ppm), 12 (47.00 ppm), 7 (46.08) ppm)

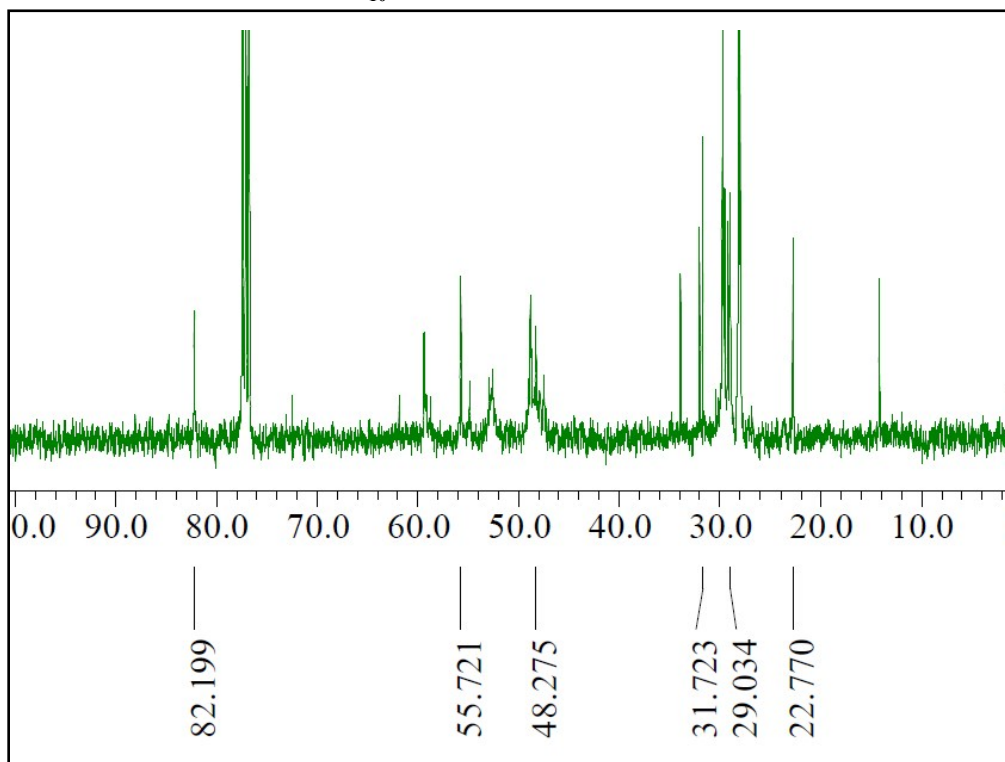
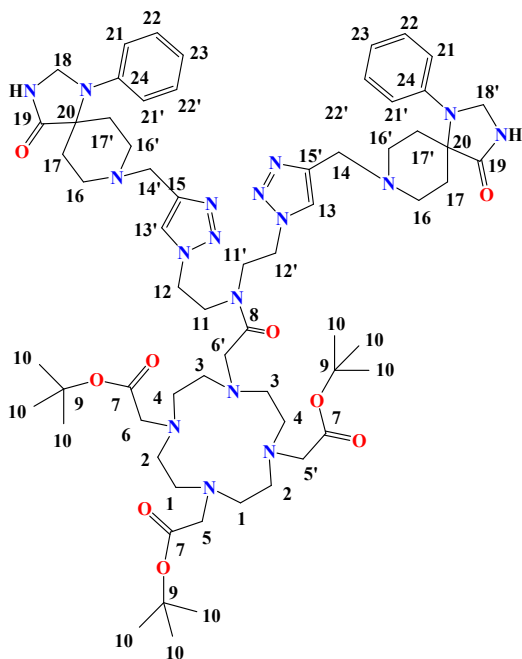
Mass Spectrum of tri-tert-butyl 2,2',2''-(10-(3-(bis(2-azidoethyl)amino)-2-oxopropyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (7)

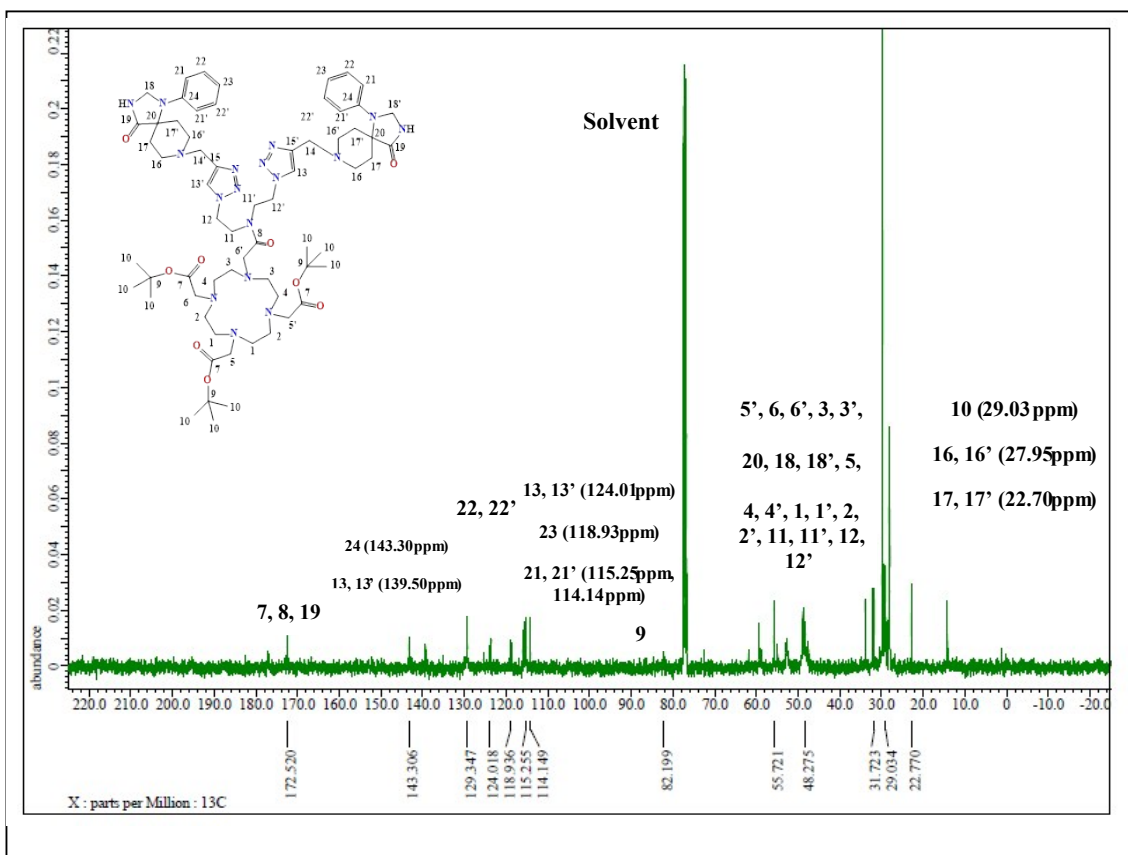


^1H NMR of tri-tert-butyl 2,2',2''-(10-(2-(bis(2-(5-((4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]decan-8-yl)methyl)-1H-1,2,3-triazol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (8),
(Solvent: CDCl_3)



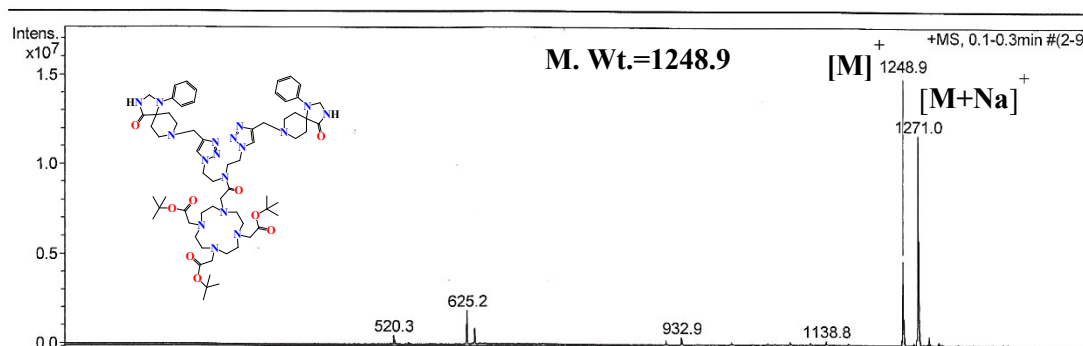
^{13}C NMR of tri-tert-butyl 2,2',2''-(10-(2-(bis(2-(5-((4-oxo-1-phenyl-1,3,8-triazaspiro [4,5]decan-8-yl)methyl)-1H-1,2,3-triazol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (8), (Solvent: CDCl_3)



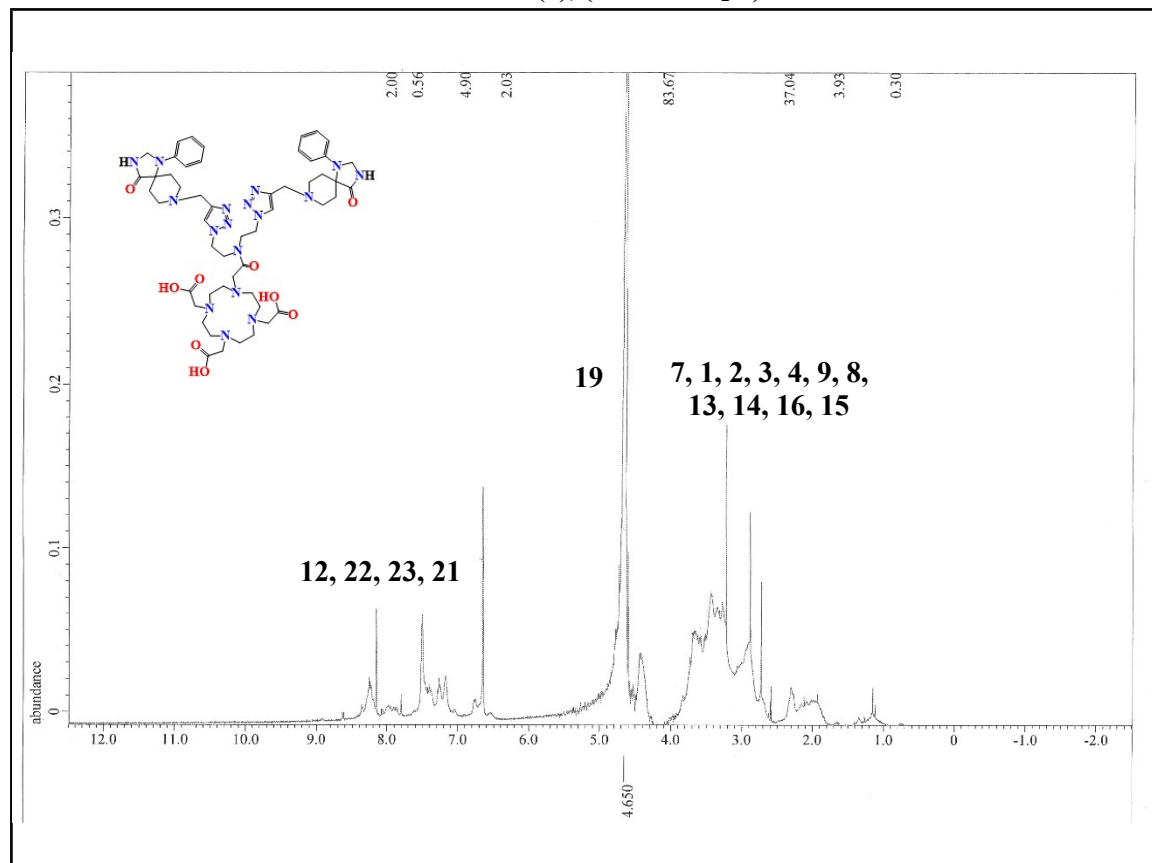


Values (ppm) = 20 (72.34); 18,18' (62.03); 5, 5' (59.65); 6, 6' (58.85); 3, 3' (55.72, 54.55); 4, 4' (53.55, 52.03); 1, 1' (49.75, 48.83); 2, 2' (48.27, 48.21); 11, 11' (57.53, 57.42); 12, 12' (31.85, 31.72)

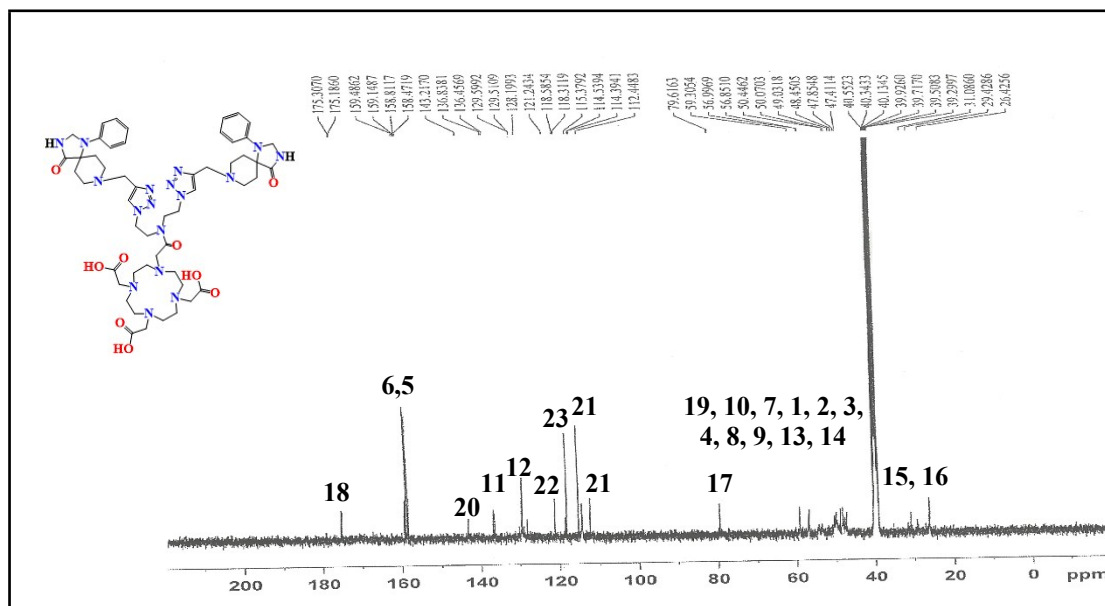
Mass Spectrum of tri-tert-butyl 2,2',2''-(10-(2-(bis(2-(5-((4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]decan-8-yl)methyl)-1,2,3-triazol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetate (8)

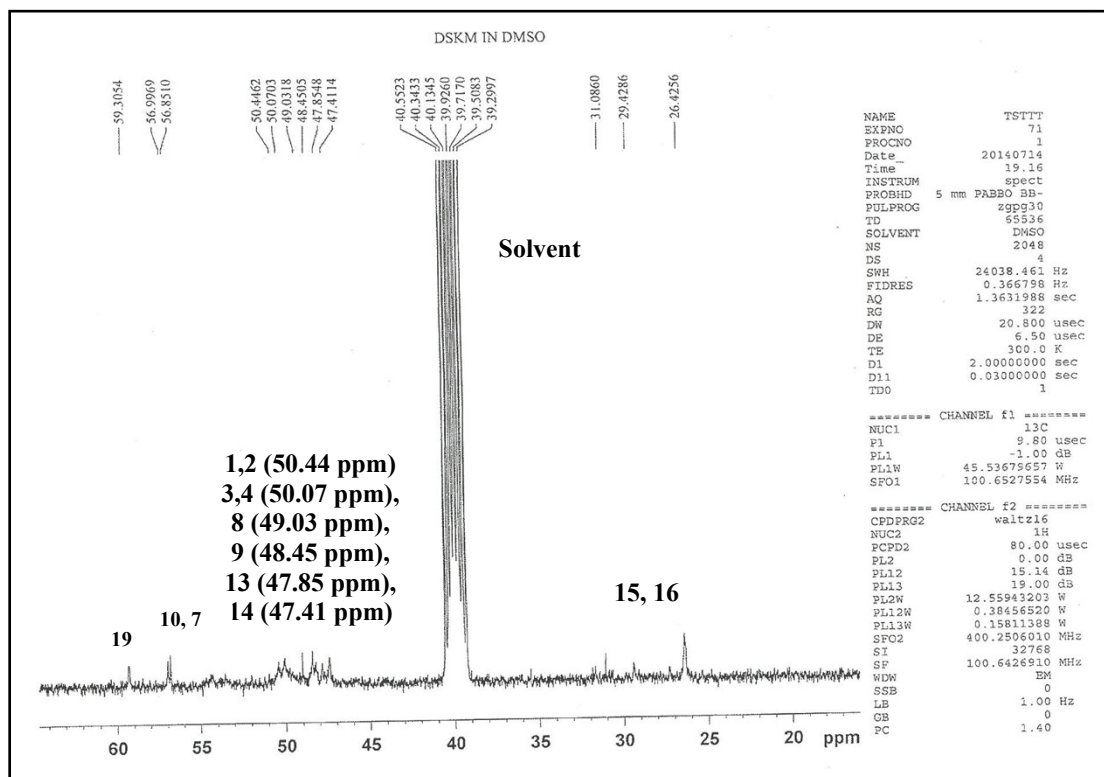
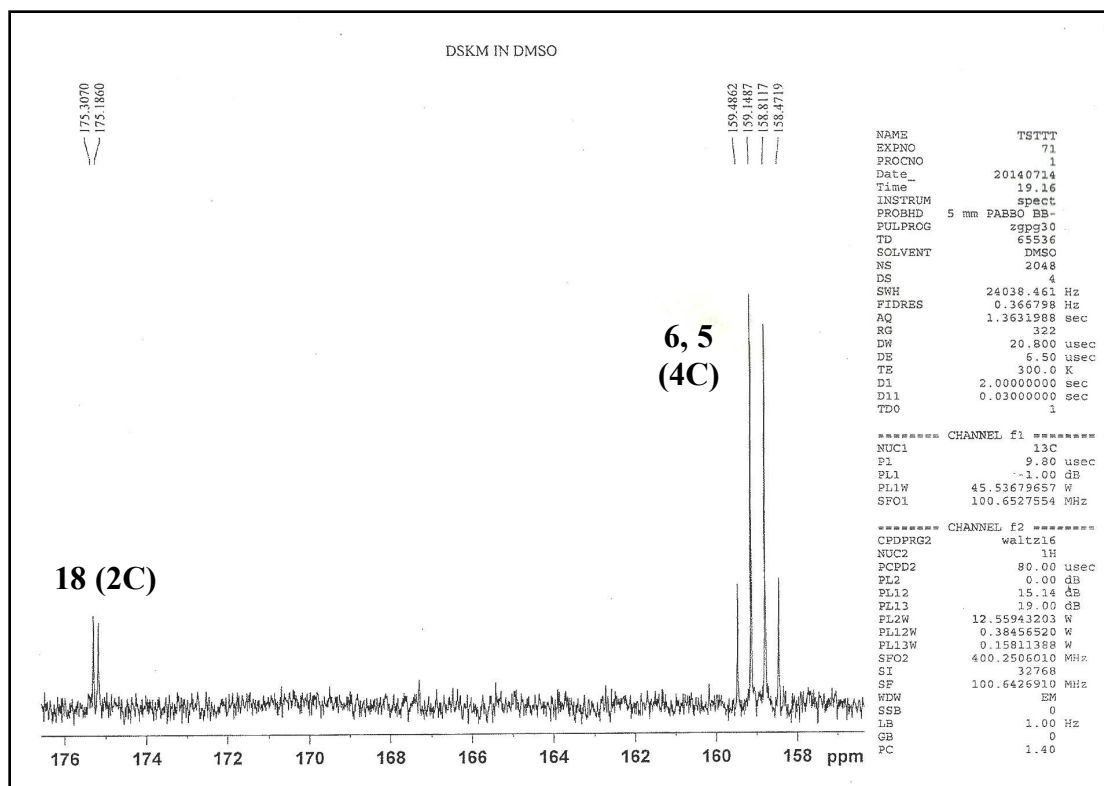


¹H NMR of 2,2',2''-(10-(2-(bis(2-(5-((4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]decan-8-yl) methyl)-1H-1,2,3-triazol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetic acid (9), (Solvent: D₂O)

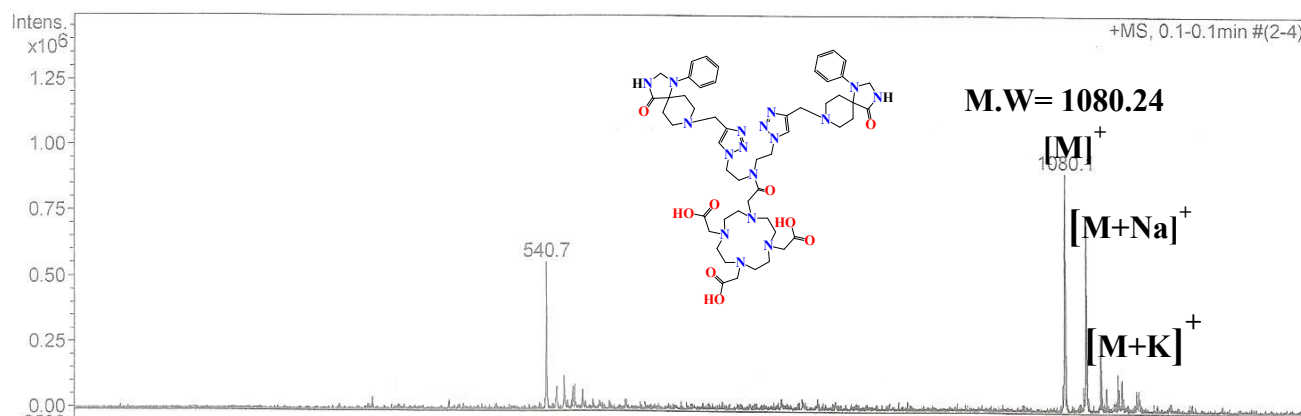


¹³C NMR of 2,2',2''-(10-(2-(bis(2-(5-((4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]decan-8-yl) methyl)-1H-1,2,3-triazol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetic acid (10)





Mass Spectrum of 2,2',2''-(10-(2-(bis(2-(5-((4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]decan-8-yl)methyl)-1H-1,2,3-triazol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetic acid
(9)



Mass Spectrum of Gadolinium loaded 2,2',2''-(10-(2-(bis(2-(5-((4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]decan-8-yl)methyl)-1H-1,2,3-triazol-1-yl)ethyl)amino)-2-oxoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triyl)triacetic acid (10)

